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Supplementary Information

Single-component solid state white-light emission and photoluminescent color tuning of a Cd(II) complex and its application as luminescent thermometer

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Table S1. Crystal data and refinement details of **1** and **3**.

Crystal data	**1**	**3**
Empirical formula	$C_{19}H_{16}CdN_2O_4$	$C_{42}H_{30}Cd_3O_{12}$
Formula weight (g ·mol^{-1})	448.74	1063.86
Temperature (K)	293.15	293(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	monoclinic	triclinic
Space group	$P2_1/n$	P-1
a (Å)	12.5936(5)	8.9832(2)
b (Å)	8.8231(3)	10.0012(4)
c (Å)	16.1379(6)	11.0442(4)
α(^{o})	90.00	76.698(3)
β (^{o})	99.837(4)	81.519(2)
γ(^{o})	90.00	78.513(3)

Volume (Å^3)	1766.78(12)	940.89(6)
Z	4	1
ρ_{calc} (Mg·m^{-3})	1.687	1.878
μ (mm^{-1})	1.263	1.746
F(000)	896.0	522.0
Crystal size (mm)	0.38 × 0.36 × 0.18	0.1 × 0.08 × 0.06
2θ range for data collection (º)	5.98 to 52.72	6.08 to 52.744
Limiting indices	-15 ≤ h ≤ 15 -10 ≤ k ≤ 11 -19 ≤ l ≤ 20	-11 ≤ h ≤ 11 -12 ≤ k ≤ 12 -13 ≤ l ≤ 13
Reflections collected/ Independent [R_{int}]	11203/3594 [R_{int} = 0.0313]	22321/3850 [R_{int} = 0.0325]
Data / restraints / parameters	3594/0/188	3850/0/259
Goodness-of-fit on F^2	1.037	1.053
Final R indices [I > 2σ(I)]	R_1 = 0.0493, wR_2 = 0.1137	R_1 = 0.0221, wR_2 = 0.0468
R indices (all data)	R_1 = 0.0632, wR_2 = 0.1242	R_1 = 0.0297, wR_2 = 0.0500
Largest diff. peak and hole (Å^{-3})	2.00/-1.13	0.84/-0.42
CCDC number	1909941	1909939

Table S2. Selected bond lengths and angles of **1**.

Bond lengths (Å)		bond angles (°)	
Cd1-O4^{i}	2.307(3)	O4-Cd1-O4^{i}	78.4(1)
Cd1-O4	2.273(3)	O4-Cd1-O3	79.6(1)
Cd1-O2	2.228(3)	O4^{i}-Cd1-O3	157.9(1)
Cd1-O3	2.359(3)	O4-Cd1-N1	98.4(1)
Cd1-N1	2.279(4)	O4^{i}-Cd1-O1	93.9(1)
Cd1-O1	2.324(4)	O4-Cd1-O1	90.1(1)
		O2-Cd1-O4	165.9(1)
		O2-Cd1-O4^{i}	112.3(1)
		O2-Cd1-O3	89.4(1)
		O2-Cd1-N1	90.5(1)
		O2-Cd1-O1	80.2(1)
		N1-Cd1-O4^{i}	92.9(1)
		N1-Cd1-O3	90.6(1)
		N1-Cd1-O1	170.1(1)
		O1-Cd1-O3	85.8(1)

^{i}symmetry code:1-x, 1-y, -z

Table S3. Selected bond lengths of **3**.

Bond lengths (Å)		Bond lengths (Å)	
Cd1-O2	2.229(2)	Cd2-O5	2.250(2)
Cd1-O3	2.310(2)	Cd2-O3	2.310(2)
Cd1-O1	2.310(2)	Cd2-O6^{1}	2.285(2)
Cd2-O2	2.281(2)	Cd2-O4	2.300(2)
Cd2-O5^{i}	2.285(2)		

^{i}symmetry code: 1-x,1-y,1-y

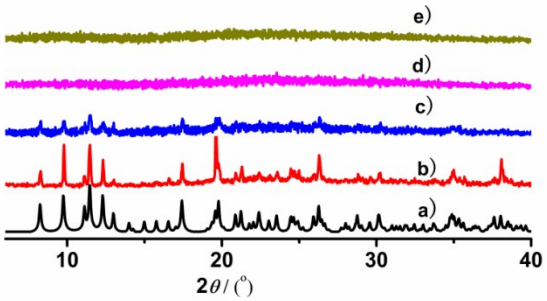

Fig. S1. PXRD patterns of **1**, a) simulated from single crystal data, b) as-synthesized, c) ground for 5 min, d) ground for 20 min, and e) heated at 180 °C (after grinding) for 20 min.

Table S4. Photophysical data of crystals of **1**.

λ_{ex} (nm)	CIE1931 chromaticity coordinate	Color temperature (K)	Quantum yield
300	0.3327, 0.3284	5472	0.13
350	0.3305, 0.3404	5579	0.17
370	0.3291, 0.3302	5648	0.15
400	0.3269, 0.3377	5753	0.15

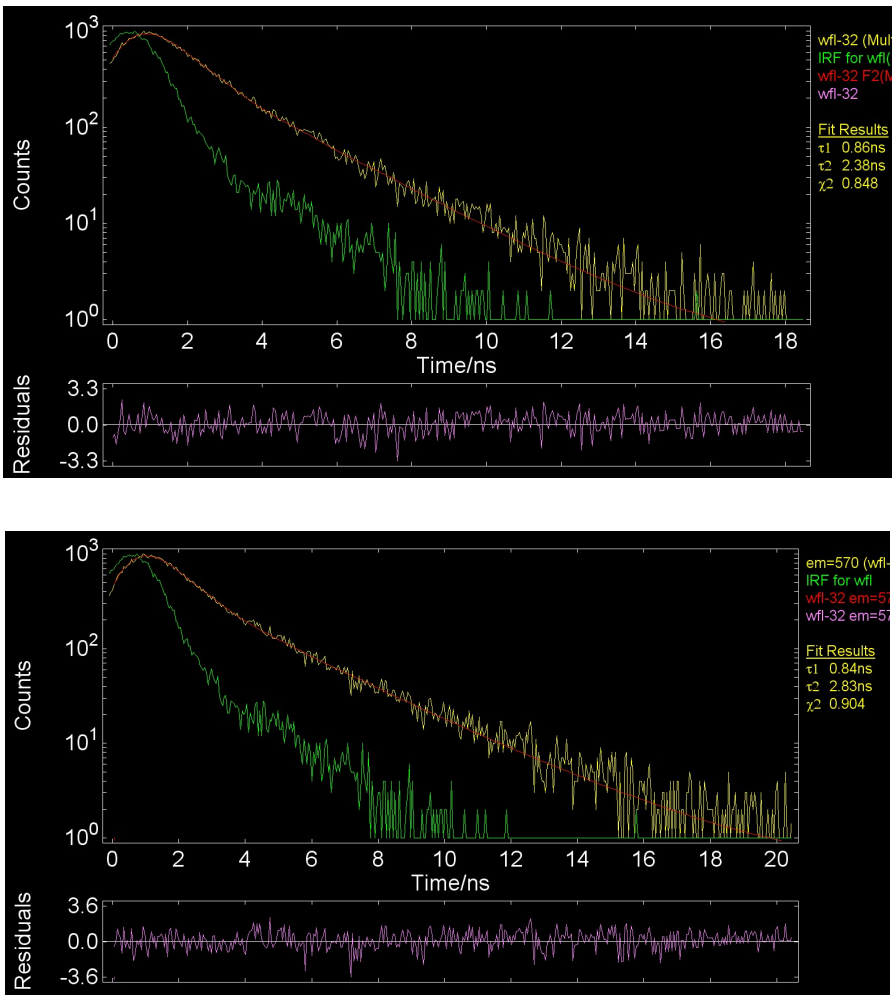

Fig. S2. Fluorescence lifetime profiles of crystals of **1** (upper: λ_{ex} = 370 nm, λ_{em} = 457 nm; bottom: λ_{ex} = 370 nm, λ_{em} = 570 nm).

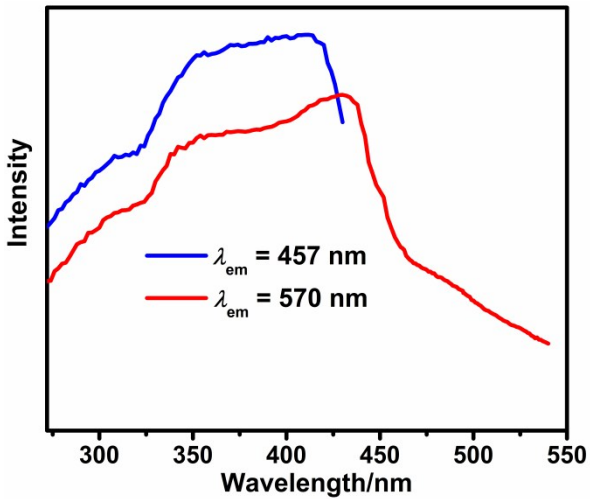

Fig. S3. Excitation spectra of crystals of **1**.

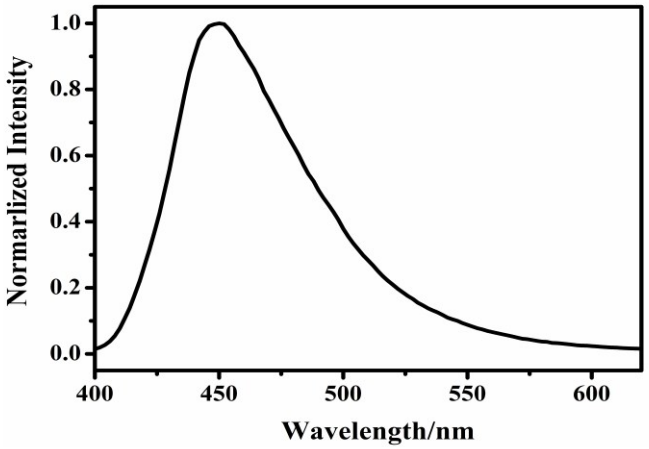

Fig. S4. Emission spectrum of **2** (λ_{ex} = 370 nm).

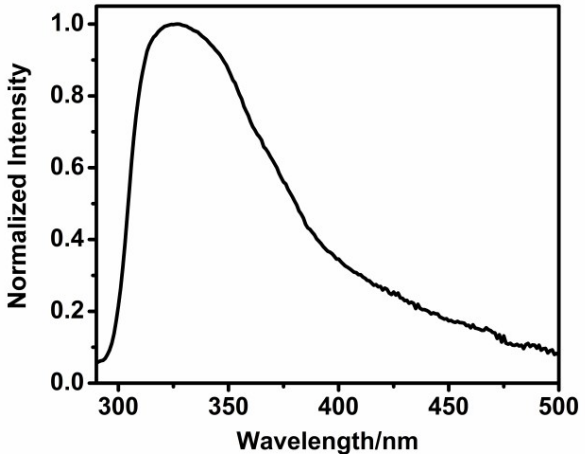

Fig. S5. Emission spectrum of $PyNH_2$ (λ_{ex} = 260 nm).

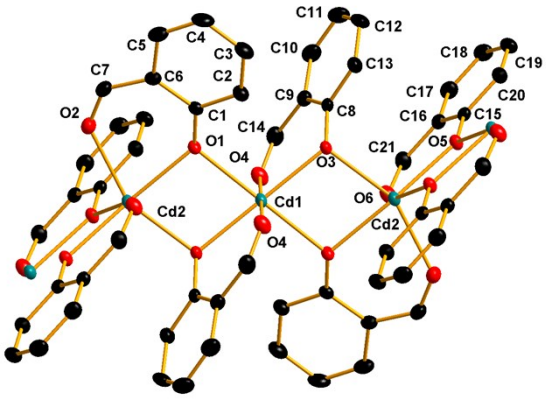

Fig. S6. Crystal structure of **3**.

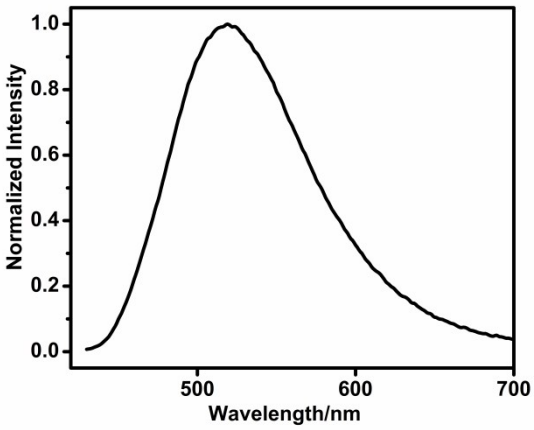

Fig. S7. Emission spectrum of **3** (λ_{ex} = 400 nm).

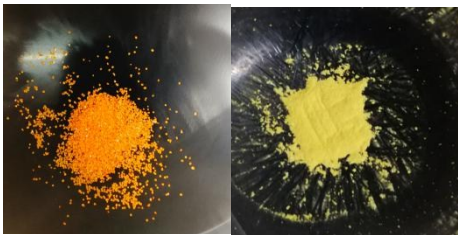

Fig. S8. Pictures of **1** before (left) and after (right) grinding under ambient light.

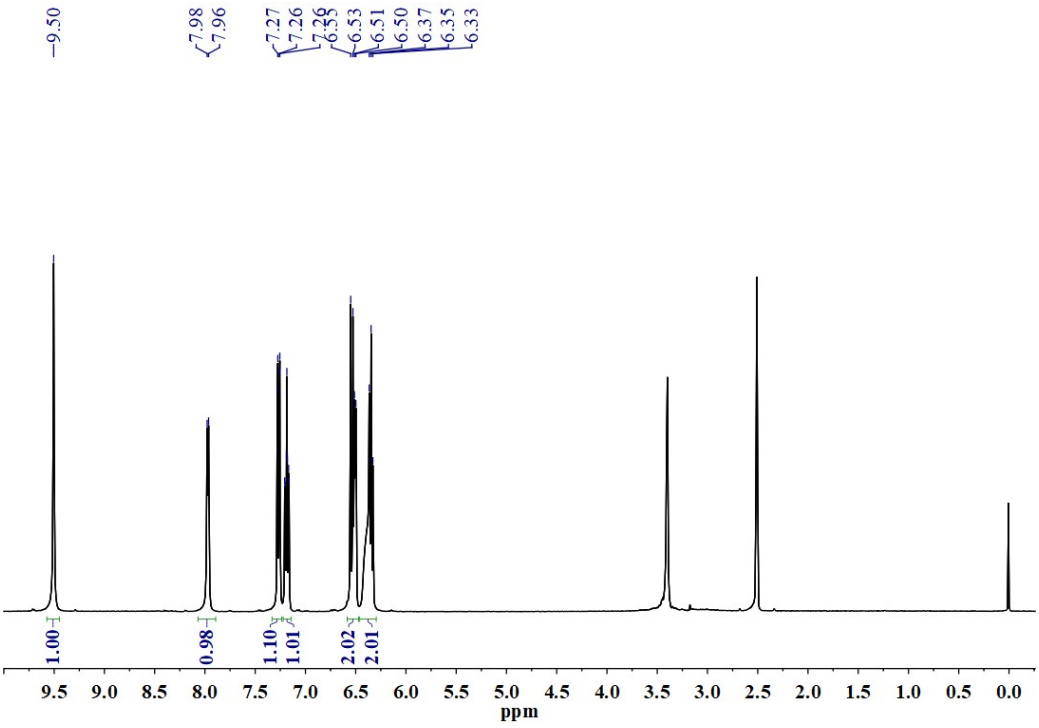

Fig. S9. ^{1}H-NMR spectrum of crystalline **1** in DMSO-d_6. δ 9.50 (s, 1H), 7.97 (d, J = 5.8 Hz, 1H), 7.27 (dd, J = 7.9, 1.9 Hz, 1H), 7.18 (ddd, J = 8.7, 6.8, 1.9 Hz, 1H), 6.64-6.41(m, 2H), 6.39-6.25 (m, 2H).

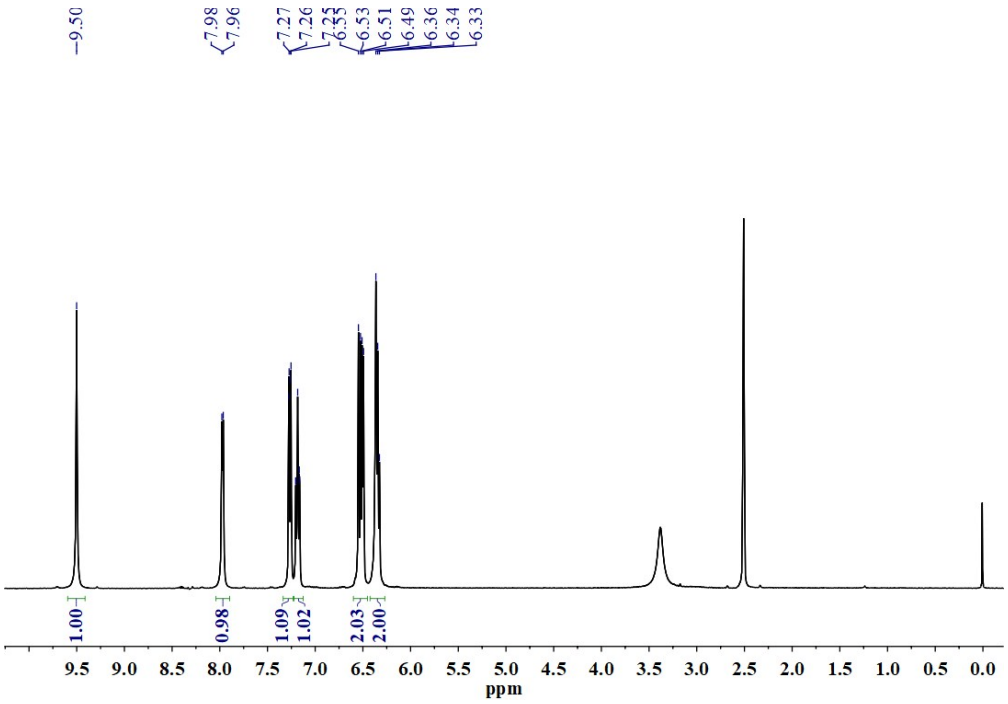

Fig. S10. ^{1}H-NMR spectrum of **1** (after being ground for 20 min) in DMSO-d_6. δ 9.50 (s, 1H), 7.97 (d, J = 5.7 Hz, 1H), 7.27 (dd, J = 7.9, 1.7 Hz, 1H), 7.21-7.12 (m, 1H), 6.64-6.40 (m, 2H), 6.39-6.29 (m, 2H).

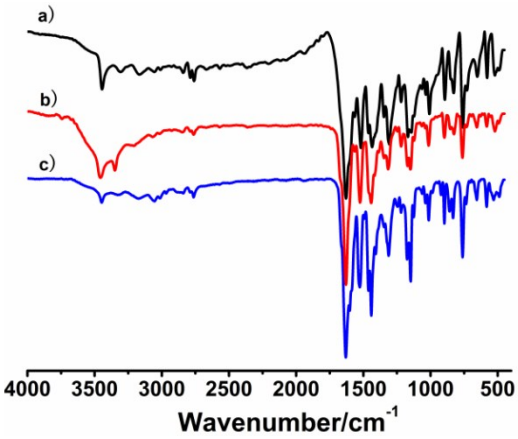

Fig. S11. FT-IR spectra of **1**, a) crystals, b) amorphous, c) amorphous sample heated at 180 °C.

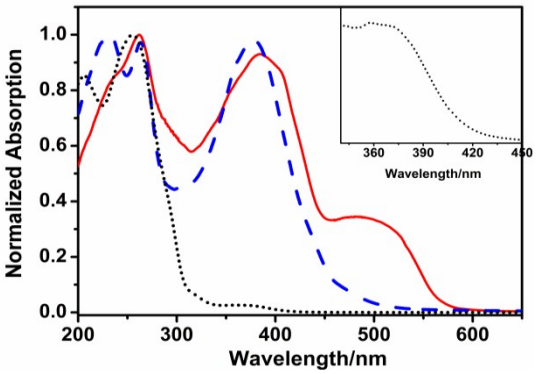

Fig. S12. Solid state absorption spectra of **1** (red line), **2** (black dotted line) and **3** (blue dashed line). Inset: the enlarged region around 370 nm of **2**.

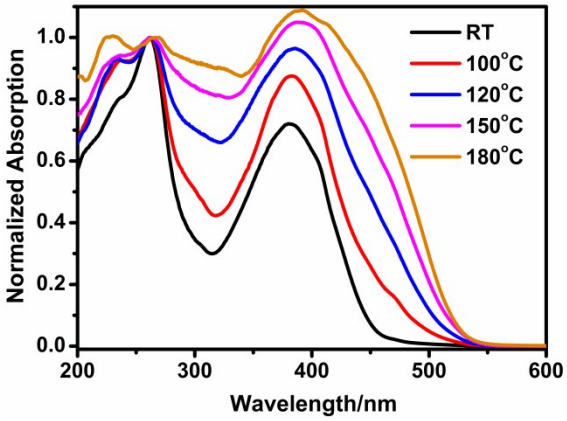

Fig. S13. Solid state absorption spectra of amorphous **1** after being heated at different temperatures.

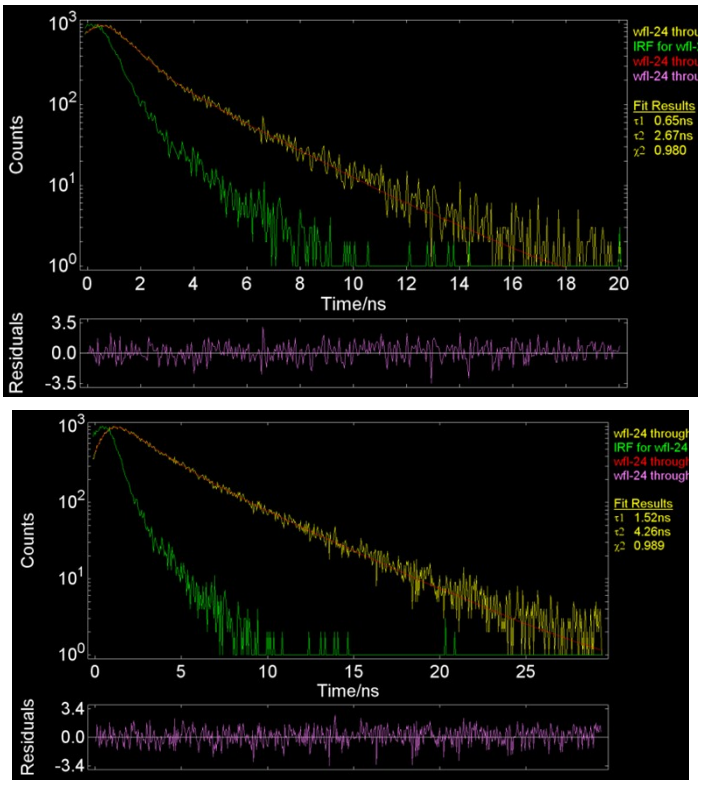

Fig. S14. Fluorescence lifetime profiles of amorphous **1** (upper: λ_{ex} = 370 nm, λ_{em} = 457 nm; bottom: λ_{ex} =370 nm, λ_{em} = 515 nm).

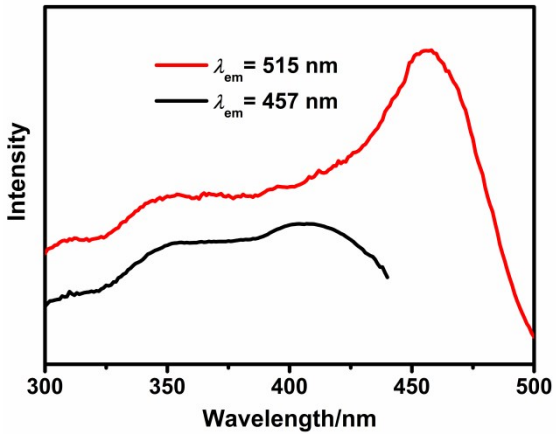

Fig. S15. Excitation spectra of amorphous **1**.

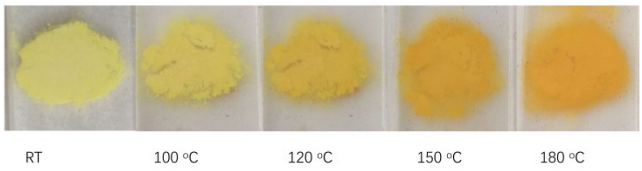

Fig. S16. Photos of amorphous **1** at different temperatures under ambient light.

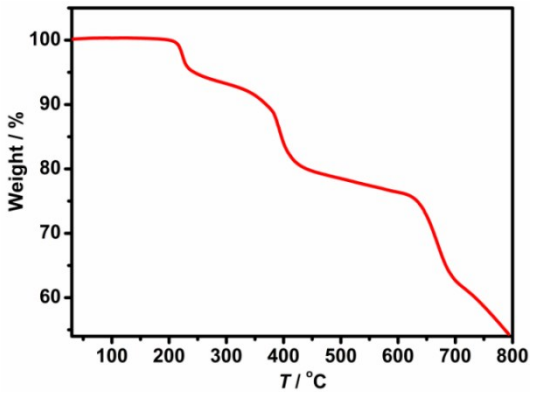

Fig. S17. TGA curve of amorphous **1**.

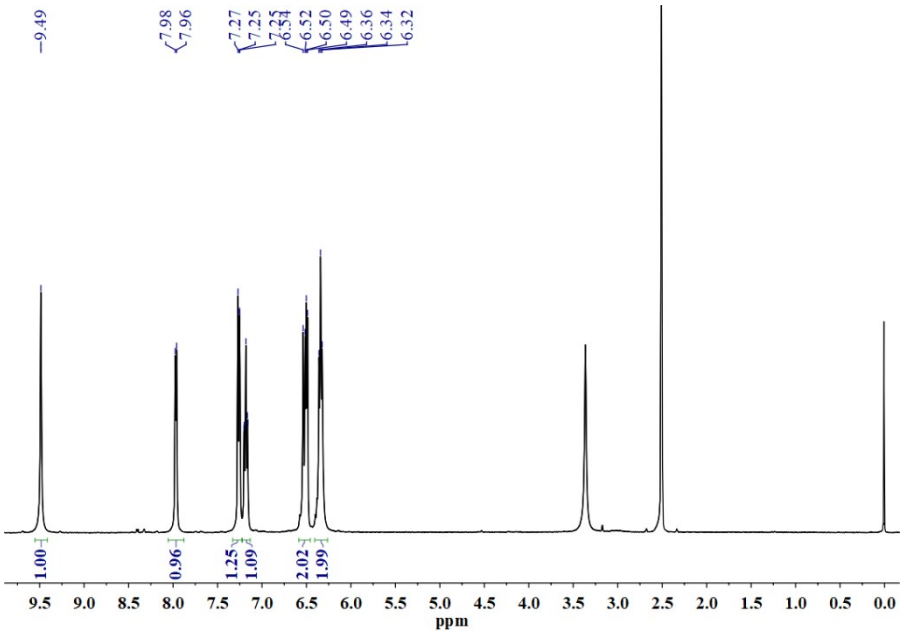

Fig. S18. ^{1}H-NMR spectrum of **1** (after being heated to 180 °C) in DMSO-d_6. δ 9.49 (s, 1H), 7.97 (d, J = 5.8 Hz, 1H), 7.27 (dd, J = 7.9, 1.9 Hz, 1H), 7.18 (ddd, J = 8.7, 6.8, 1.9 Hz, 1H), 6.63-6.41 (m, 2H), 6.39-6.29 (m, 2H).

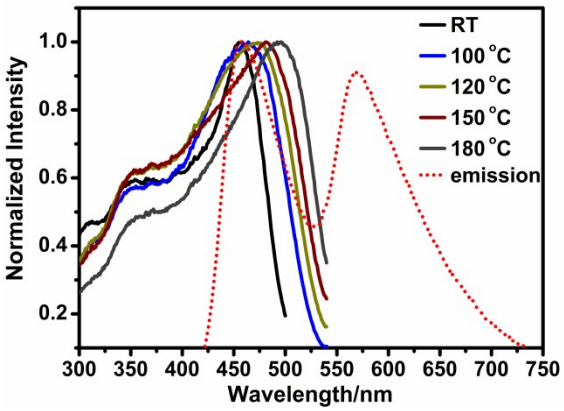

Fig. S19. Emission spectrum of crystalline **1** (red dotted line), and excitation spectra of amorphous **1** (solid lines) at different temperatures.